Anomalous conductance in trans-polyacetylene chains with even-odd parity

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Low-dimensionality systems, such as conjugated polymers, have been extensively investigated, allowing the study of essential aspects of quantum mechanics, structural properties and transport of electronic devices [1]. Thus, the investigation of atomic chains in experiments and theories has become one of the central topics of the science of nanomaterials [2]. This work presents an analytical study of the electron transport characteristics of dimerized trans-polyacetylene (trans-PA) molecules containing an even and odd number of sites coupled to metal electrodes (left and right) with T-shaped geometry using the Su-Schrieffer-Heeger (SSH)[3] described by the tight-binding Hamiltonian, through the Heisenberg equation of motion and electron transport through the Non-equilibrium Green function method and Keldysh formalism[4]. Our proposal was to test the effects on the finite-size chain for three, four, and five sites and, furthermore, predicted for 17 sites via current-voltage effects and the degree of chain dimerization. (I) The dimerization forces (δ) for odd chain is the electronic transport channel, (ii) and for even chains the oscillations present in the electronic transport via conductance are dependent on the size of the nanowire and also sensitive to the dimerization force. In fact, this corroborates in the transport dynamics for different degrees of dimerized topological chains since; the interaction of these two factors allows transitions of the metal-semiconductor type.

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